

Solution of electric-field-driven tight-binding lattice in contact with fermion reservoirs

Jong E. Han

Department of Physics, State University of New York at Buffalo, Buffalo, New York 14260, USA

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Electrons in tight-binding lattice driven by DC electric field dissipate their energy through on-site fermionic thermostats. Due to the translational invariance in the transport direction, the problem can be block-diagonalized. We solve this time-dependent quadratic problem and demonstrate that the problem has an oscillatory steady-state. The steady-state occupation number shows that the Fermi surface disappears for any damping from the thermostats and any finite electric field. Despite the lack of momentum scattering, the conductivity takes the same form as the semi-classical Ohmic expression from the relaxation-time approximation.

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I. INTRODUCTION

Nonequilibrium phenomena in lattice is one of the oldest and most fundamental problems in solid state physics. In conventional solids, the acceleration due to external field is relatively small compared to electronic energy, and various scattering mechanisms make the transport diffusive enough so that the small field approximation has often been used. The quantum Boltzmann method has been applied effectively^{1,2} and linear response limit has been widely used in the literature. However, recent progress in nano-devices and optical lattice systems has made rigorous high-field formalism necessary to understand their non-perturbative effects such as the Bloch oscillation. In such regime, understanding the interplay of non-perturbative field-effect and the many-body physics has emerged as one of the most pressing problems in nano-science.

Combining the nonequilibrium and quantum many-body effects is an extremely challenging task. Much effort has been exerted towards understanding strong correlation physics in quantum dot physics, especially the nonequilibrium Kondo problem. Analytical theories³⁻⁵ and many numerical methods have been proposed along the time-dependent⁶⁻⁸, and steady-state simulations^{10,11}. In such systems with localized interacting region, the important question of energy dissipation could have been side-stepped, and the existence of steady-state has not been a major issue.

In the past few years, non-perturbative inclusion of electric-field and many-body effects has been one of the important issues in the field. Theories for lattice nonequilibrium have been formulated^{12,13}, mostly based on the dynamical mean-field theory (DMFT) for an *s*-orbital tight-binding (TB) lattice with on-site interaction¹⁴⁻¹⁷. Although a long-held belief in solid-state transport has been that, under a finite electric-field, the Fermi sea is *perturbatively* shifted by a drift velocity, many calculations performed under the DMFT framework have suggested that the system approaches a steady-state with infinitely hot electron gas even for small field. With inclusion of proper dissipation mechanism, correct models should expect the Boltzmann picture of displaced Fermi

surface at small fields and a recovery of the Bloch oscillation in the high-field limit.

However, it is unclear so far which of the approximations, such as single-band approximation without Landau-Zener tunneling or the nature of on-site interaction, are responsible for the rather peculiar long-time states. One of the goals of this paper is that we provide exact solutions to one of the dissipation models with on-site fermion thermostats and give analytic understanding of the problem, and guide possible future modeling.

Due to the nature of the one-body reservoirs, the problem can be solved exactly (see Fig. 1). With identical reservoirs on each site, the Hamiltonian can be block-diagonalized according to the wave-vector of electrons in the transport direction. The block-diagonal Hamiltonian can then be exactly solved by a time-dependent perturbation theory^{18,19} using the nonequilibrium Green function theory. The calculation of the occupation number supports the numerical observations that the Fermi surface of the unperturbed equilibrium is completely lost with effectively infinite temperature, in contrast to the conventional picture of the displaced Fermi sea under finite electric field. Despite the lack of momentum scattering, the DC electric current of this model recovers the familiar semi-classical Boltzmann equation result²⁰.

II. MODEL

We study a quadratic model of a one-dimensional *s*-orbital tight-binding model connected to fermionic reservoirs (see Fig. 1) under a uniform electric field E . The effect of the electric field is absorbed in the temporal gauge as the Peierls phase $\varphi(t) = eEat$ to the hopping integral¹² γ . The time-dependent Hamiltonian then reads

$$\begin{aligned} \hat{H}(t) = & -\gamma \sum_i (e^{i\varphi(t)} d_{i+1}^\dagger d_i + H.c.) + \sum_{i\alpha} \epsilon_\alpha c_{i\alpha}^\dagger c_{i\alpha} \\ & -g \sum_{i\alpha} (c_{i\alpha}^\dagger d_i + H.c.), \end{aligned} \quad (1)$$

with d_i^\dagger as the (spinless) electron operator on the tight-binding chain on site i , $c_{i\alpha}^\dagger$ with the reservoir fermion

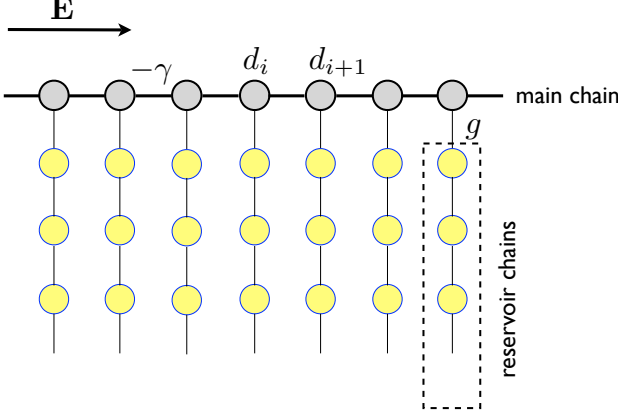


FIG. 1: One-dimensional tight-binding lattice of orbital d_i under an electric field E . Each lattice site is connected to an identical fermionic bath of $\{c_{i\alpha}\}$ with the continuum index α along the reservoir chain direction.

states connected to the site i with the continuum index α along each reservoir chain. Here we do not specify the explicit connectivity of the reservoir chains, but each chain is assumed to have an identical dispersion relation ϵ_α . Notice that the electric field is applied only on the tight-binding chain $\{d_i^\dagger\}$. The coupling between the TB site and the reservoir is given by the identical tunneling parameter g . The Peierls phase $\varphi(t)$ is given as

$$\varphi(t) = \begin{cases} 0, & \text{for } t < 0 \\ \Omega t, & \text{for } t > 0 \end{cases} \quad (2)$$

$\Omega = eEa$ is the Bloch-oscillation frequency due to the electric field.

We note that the whole system has discrete translational symmetry in the transport direction and the Hamiltonian is readily block-diagonalized with respect to the wave-vector k as $d_k^\dagger = \sqrt{N_d^{-1}} \sum_j e^{ikR_j} d_j^\dagger$ and $c_{k\alpha}^\dagger = \sqrt{N_d^{-1}} \sum_j e^{ikR_j} c_{j\alpha}^\dagger$ (with lattice sites $R_j = aj$ and the number of sites along the TB chain N_d),

$$\hat{H}(t) = \sum_k \left[-2\gamma \cos(k + \varphi(t)) d_k^\dagger d_k + \sum_\alpha \epsilon_\alpha c_{k\alpha}^\dagger c_{k\alpha} - g \sum_\alpha (c_{k\alpha}^\dagger d_k + H.c.) \right]. \quad (3)$$

Here $\epsilon_d(k) = -2\gamma \cos(k)$ is the tight-binding dispersion at zero E -field. Then each k -sector can be treated and solved separately. So from now on, we suppress the k -subscript until necessary with the following Hamiltonian,

$$\hat{H}_k(t) = -2\gamma \cos(k + \varphi(t)) d^\dagger d + \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha - g \sum_\alpha (c_\alpha^\dagger d + H.c.). \quad (4)$$

It is important to note that the k -dependence enters the problem as $k + \varphi(t)$ for $t > 0$. This problem is simply a resonant level model¹⁸ where the level is modulated sinusoidally for $t > 0$. Considering these two observations, we can infer that different k only adds different phase to $k + \varphi(t)$ and steady-state properties such as the average occupation number $n_k(t) = \langle d^\dagger(t) c(t) \rangle$ are expected to be k -independent. This shows that the on-site fermion thermostat problem completely obliterates the Fermi surface at any non-zero field and, even in the small damping limit, and does not restore the conventional picture of shifted Fermi surface due to an external field.

III. SOLUTION FOR OCCUPATION NUMBER AND CURRENT

The time-dependent Hamiltonian (4) can be exactly solved by the nonequilibrium Keldysh Green function method¹⁹. We write the Hamiltonian as $\hat{H}_k(t) = \hat{H}_0 + \hat{V}(t)$ with the time-independent unperturbed part $\hat{H}_0 = \hat{H}_k(0)$ and the time-dependent perturbation as $\hat{V}(t) = \hat{H}_k(t) - \hat{H}_k(0)$,

$$\hat{V}(t) = -2\gamma [\cos(k + \varphi(t)) - \cos(k)] d^\dagger d \equiv v(t) d^\dagger d. \quad (5)$$

When the perturbation is one-body on discrete states the lesser and greater part of the self-energy is zero, and the lesser d -Green function $G^<$ is expressed only in terms of the transient term, symbolically written as¹⁹

$$G^< = [I + G^r V] G_0^< [I + V G^a] \quad (6)$$

and the retarded Green function G^r is given by the usual Dyson's equation

$$G^r = G_0^r + G_0^r V G^r, \quad (7)$$

where the matrix product means convolution-integrals in time.

First with the retarded functions, the non-interacting limit has the time-translational symmetry and

$$\begin{aligned} G_0^r(t - t') &= -i\theta(t - t') \int_{-\infty}^{\infty} d\epsilon \frac{\Gamma/\pi}{\epsilon^2 + \Gamma^2} e^{-i\epsilon(t-t')} \\ &= -i\theta(t - t') e^{-i\epsilon_d(k)(t-t') - \Gamma|t-t'|}, \end{aligned} \quad (8)$$

where we use a flat-band DOS for the reservoir in the infinite-band limit with the hybridization broadening $\Gamma = \pi g^2 N(0)$ and the density of states of the fermion bath $N(0) = \sum_\alpha \delta(\epsilon_\alpha)$. Writing $G^r(t, t') = G_0^r(t - t') g^r(t, t')$, Eq. (7) becomes

$$g^r(t, t') = 1 - i \int_{t'}^t ds v(s) g^r(s, t'), \quad (9)$$

which can be solved as

$$g^r(t, t') = \exp \left[-i \int_{t'}^t v(s) ds \right], \quad (10)$$

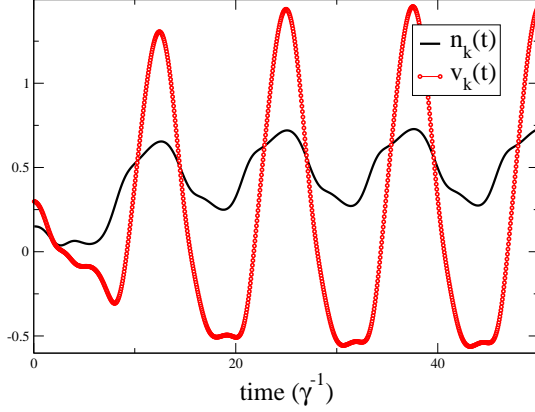


FIG. 2: Expectation value of occupation number $n_k(t)$ of wave-vector k and the current $J_k(t)$ for $\gamma = 1$, $\Omega = 0.5$, $\Gamma = 0.1$ and at $k = \pi/2 + 0.1$. After the initial time of Γ^{-1} , transient behavior dies out and the expectation values reach steady oscillation.

and finally we have for the full retarded Green function

$$G^r(t, t') = -i\theta(t-t')e^{-i\epsilon_d(k)(t-t')-\Gamma|t-t'|} \exp\left[-i\int_{t'}^t v(s)ds\right] \quad (11)$$

For the same-time argument for $G^<$ we have the Dyson's equation

$$\begin{aligned} G^<(t, t) &= G_0^<(t, t) \\ &+ \int_0^t [G^r(t, s)v(s)G_0^<(s, t) + G_0^<(t, s)v(s)G^a(s, t)] ds \\ &+ \int_0^t \int_0^t G^r(t, s)v(s)G_0^<(s, s')v(s')G^a(s', t)dsds'. \end{aligned} \quad (12)$$

We set the initial lesser Green function with the half-filled reservoir at zero temperature as

$$G_0^<(t, t') = i \int_{-\infty}^0 d\omega \frac{\Gamma/\pi}{(\omega - \epsilon_d(k))^2 + \Gamma^2} e^{-i\omega(t-t')}. \quad (13)$$

After some straightforward steps, the occupation number for the wave-vector k , $n_k(t) = -iG^<(t, t)$, becomes

$$\begin{aligned} n_k(t) &= \int_{-\infty}^0 d\omega \frac{\Gamma/\pi}{(\omega - \epsilon_d(k))^2 + \Gamma^2} \times \\ &\left| 1 - i \int_0^t ds v(s) e^{i(\omega - \epsilon_d(k) + i\Gamma)(t-s) - i \int_s^t v(s')ds'} \right|^2. \end{aligned} \quad (14)$$

Fig. 2 shows the above $n_k(t)$ numerically evaluated for $\gamma = 1$, $\Omega = 0.5$, $\Gamma = 0.1$ and at $k = \pi/2 + 0.1$. Due to the exponential factor $e^{-\Gamma(t-s)}$, the integral converges to a steady-state oscillation state after time $t \approx \Gamma^{-1}$ and the transient behavior dies out. Therefore, for long-time behavior, the time-integral range $[0, t]$ can be changed to

$[-\infty, t]$ for easier analytic treatment. After an integral-by-parts and some straightforward steps, we have

$$\begin{aligned} n_k(t) &= \frac{\Gamma}{\pi} \int_{-\infty}^0 d\omega \times \\ &\left| \int_{-\infty}^0 ds e^{-i(\omega + i\Gamma)s - i(2\gamma/\Omega) \sin(k + \Omega(t+s))} \right|^2. \end{aligned} \quad (15)$$

An identity for Bessel functions $J_n(x)$

$$e^{ix \cos \theta} = \sum_{m=-\infty}^{\infty} i^m J_m(x) e^{im\theta} \quad (16)$$

can be used to perform the integrals as

$$\begin{aligned} n_k(t) &= \frac{\Gamma}{\pi} \sum_{nm} \frac{J_n(\frac{2\gamma}{\Omega}) J_m(\frac{2\gamma}{\Omega}) e^{i(m-n)(k+\Omega t)}}{-(m-n)\Omega + 2i\Gamma} \times \\ &\left[\frac{1}{2} \log \frac{m^2\Omega^2 + \Gamma^2}{n^2\Omega^2 + \Gamma^2} + i\chi_{mn} \right] \end{aligned} \quad (17)$$

with

$$\chi_{mn} = \pi + \tan^{-1} \frac{m\Omega}{\Gamma} + \tan^{-1} \frac{n\Omega}{\Gamma}. \quad (18)$$

As pointed out earlier, it is important to note that the k and t -dependence is only in the exponential factor as $e^{i(m-n)(k+\Omega t)}$. Therefore, taking a time-average over the period $2\pi\Omega^{-1}$ gives k -independent results, which have been confirmed in numerical calculations. For instance, the DC limit of $n_k(t)$ only involves the terms of $m = n$ in Eq. (17), and we have

$$\bar{n}_k = \frac{1}{2} \sum_{m=-\infty}^{\infty} \left[J_m\left(\frac{2\gamma}{\Omega}\right) \right]^2 = \frac{1}{2}. \quad (19)$$

For electronic models without thermostats, it has been argued that the effective electron temperature quickly becomes infinity¹⁴ from k -independent occupation number \bar{n}_k . The same conclusion applies to this model with on-site fermionic thermostats.

Now we turn to the calculation of electric current,

$$J_k(t) = \frac{\partial \epsilon_d(k + \Omega t)}{\partial k} n_k(t) = 2\gamma \sin(k + \Omega t) n_k(t). \quad (20)$$

Due to the sine-function, the DC current has contributions only from $m - n = \pm 1$ in Eq. (17). After some manipulations, we have

$$\begin{aligned} \bar{J}_k &= \frac{2\gamma\Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m\left(\frac{2\gamma}{\Omega}\right) J_{m-1}\left(\frac{2\gamma}{\Omega}\right) \times \\ &\left[\Gamma \log \frac{m^2\Omega^2 + \Gamma^2}{(m-1)^2\Omega^2 + \Gamma^2} + \Omega\chi_{m,m-1} \right]. \end{aligned} \quad (21)$$

As in the case for $n_k(t)$, the DC limit of $J_k(t)$ becomes independent of k . The total current is shown in Figs. 3

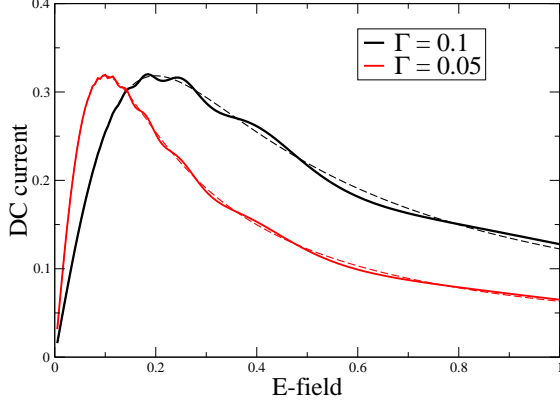


FIG. 3: DC current as a function of the damping Γ and electric field $\Omega = eEa$. For small field, the current has a linear dependence on the E -field showing an Ohm's law-like behavior. As E increases, the Bloch oscillation behavior takes over and the DC current decreases. The dashed lines are the simplified expression, Eq. (22).

and 4. Similar plot has been obtained in the interacting model from numerical calculation of Hubbard model connected to fermion bath¹⁶.

It is instructive to simplify the above expression in the limit of $\Omega, \Gamma \ll \gamma$ where the DC current is reduced to the expression

$$\bar{J} \approx \frac{4\gamma\Gamma\Omega}{\pi(\Omega^2 + 4\Gamma^2)}. \quad (22)$$

Detailed derivation is provided in Appendix. This approximate expression is shown as dashed lines in Fig. 3. Despite that the formula was derived for $\Omega, \Gamma \ll \gamma$, it shows remarkable accuracy to the DC current for a wide range of Γ and E .

It is also interesting to note that a similar formula has been derived for a super-lattice system with Ohmic scattering within the semi-classical Boltzmann transport equation²⁰. Although the current has the same dependence on the damping and the electric field, it should be emphasized that the two models have quite different scattering mechanism where in the Boltzmann approach²⁰ the momentum relaxation is explicitly built-in while in our case the lattice wave-vector scattering does not happen and a very different Fermi surface structure results. In the low-field limit, the current (22) recovers the form of the Drude conductivity per electron,

$$\bar{J} \approx \frac{\gamma\Omega}{\pi\Gamma} \propto \frac{E\tau}{m^*}, \quad (23)$$

with $\gamma \sim 1/m^*$ and $\Gamma \sim 1/\tau$.

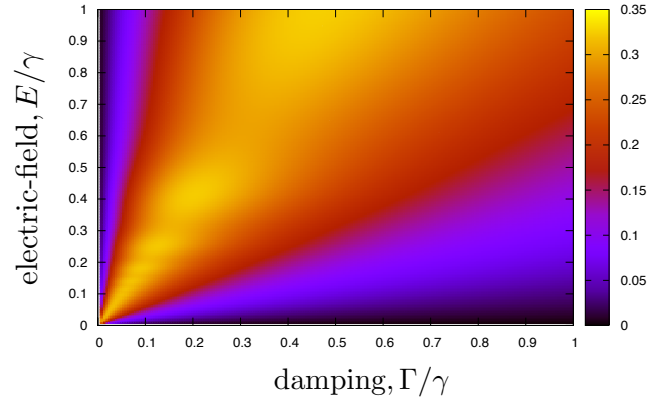


FIG. 4: Contour plot of DC current as a function of damping and electric field.

IV. CONCLUSIONS

Calculations on electron transport with fermionic thermostat confirm salient features of numerical results, such as uniform occupation number for all k -vectors in the Brillouin zone and the Ohmic-like limit of electric current. In particular, the simplified electric current, Eq. (22), recovered the semi-classical Boltzmann transport result. However, the nature of the oscillatory steady-state is quite different from the conventional solid-state transport picture. In the presence of a static electric field, this model predicts that the Fermi surface completely disappears for any finite damping Γ and electric field E after the time-evolution of the interval $\Delta t \gtrsim \max(\Omega^{-1}, \Gamma^{-1})$. The applicability of this model may be justified for studies on short-time dynamics and dissipation. However, using this model to study the strongly correlated nonequilibrium steady-state requires much caution since the uniform on-site coupling to reservoirs does not seem to preserve the Fermi surface.

We may speculate what could be the minimal elements for a realistic model which may bridge the conventional picture of Fermi surface shift and the non-perturbative field-effect, hence eventually accessing the nonequilibrium strongly correlated steady-state. One may consider momentum scattering (i) in phononic Ohmic bath (ii) in fermionic bath with site-disorder and (iii) Landau-Zener tunneling in multi-band dispersion.

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Appendix A: Derivation of current at small field

For both $\Gamma, \Omega \ll \gamma$, we expand Eq. (21) to the leading order of m as,

$$\bar{J}_k \approx \frac{2\gamma\Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m \left(\frac{2\gamma}{\Omega} \right) J_{m-1} \left(\frac{2\gamma}{\Omega} \right) \times \left[\frac{2m\Gamma\Omega^2}{m^2\Omega^2 + \Gamma^2} + 2\Omega \tan^{-1} \frac{m\Omega}{\Gamma} \right]. \quad (\text{A1})$$

Rearranging the summation and using the identity $x[J_{m-1}(x) + J_{m+1}(x)] = 2mJ_m(x)$, we write

$$\begin{aligned} \bar{J}_k &\approx \frac{2\gamma\Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m [J_{m-1} + J_{m+1}] \times \\ &\quad \left[\frac{m\Gamma\Omega^2}{m^2\Omega^2 + \Gamma^2} + \Omega \tan^{-1} \frac{m\Omega}{\Gamma} \right] \\ &= \frac{2\Gamma\Omega}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m m\Omega J_m^2 \left(\frac{m\Gamma\Omega}{m^2\Omega^2 + \Gamma^2} + \tan^{-1} \frac{m\Omega}{\Gamma} \right). \end{aligned} \quad (\text{A2})$$

For $\Omega \ll \gamma$, we define $x = m\Omega$ in the regime $m = x/\Omega \gg 1$, the summation becomes

$$\int_{-\infty}^{\infty} x J_{\frac{x}{\Omega}} \left(\frac{2\gamma}{\Omega} \right)^2 \left(\frac{x\Gamma}{x^2 + \Gamma^2} + \tan^{-1} \frac{x}{\Gamma} \right) \frac{dx}{\Omega}.$$

Using the asymptotic expression²¹ for $x/\Omega, \gamma/\Omega \rightarrow \infty$,

$$\left[J_{\frac{x}{\Omega}} \left(\frac{2\gamma}{\Omega} \right) \right]^2 \sim \begin{cases} \frac{\Omega/2\gamma}{\pi\sqrt{1-(x/2\gamma)^2}} & (|x| < 2\gamma) \\ 0 & (|x| > 2\gamma) \end{cases},$$

the integral simplifies to

$$\int_{-2\gamma}^{2\gamma} \frac{1}{\pi\sqrt{4\gamma^2 - x^2}} \left(\frac{x^2\Gamma}{x^2 + \Gamma^2} + x \tan^{-1} \frac{x}{\Gamma} \right) dx.$$

In the limit $\Gamma \ll \gamma$, the second term in the parenthesis dominates and we have

$$\bar{J} \approx \frac{2\Gamma\Omega}{\pi(\Omega^2 + 4\Gamma^2)} \int_0^{2\gamma} \frac{x dx}{\sqrt{4\gamma^2 - x^2}} = \frac{4\gamma\Gamma\Omega}{\pi(\Omega^2 + 4\Gamma^2)}. \quad (\text{A3})$$

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